Scheduling of Heat Integrated Multipurpose Batch Processes

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Abstract

A systematic mathematical framework for scheduling the operation of multipurpose batch plants involving heat-integrated unit operations is presented. The approach advocated takes direct account of the trade-offs between maximal exploitation of heat-integration and others scheduling objectives and constraints. In this paper, heat transfer takes place directly between the fluids undergoing processing in the heat integrated unit operations, and therefore a degree of time overlap of these operations must be ensured. The modelling is based on the *ERTN* formalism and a discrete time *MILP* formulation.

Key-words : Scheduling of batch processes, heat integration, *ERTN* modeling, *MILP* formulation.

1. Introduction

Recent works have highlighted the need for efficient utilization of energy in the operation of batch plants. However, in contrast to the extensive amount of work already published on energy integration in continuous plant, relatively little has been reported in the literature on this aspect of the operation and design of flexible multipurpose batch plants. The majority of studies are based on the concept of *pinch* (Linnhoff *et al*, 1988), modified in order to accommodate the complications introduced by the time-varying operation of batch processes (*Time Average Model)*. Despite its clear importance, the minimization of the cost of external utilities consumed is not usually the primary objective in scheduling the operation of a multipurpose plant. This is the consequence partly of the paramount demand for timely satisfaction of the multiple production requirements imposed on these plants and partly of the often small proportion of energy costs compared to the high value of the raw material and products produced in many such plants (e.g. ., in the pharmaceutical industry). It could, therefore, be argued that optimizing the exploitation of any heat integration opportunities afforded by a fixed production schedule that already achieves all other plant objectives is indeed a reasonable approach.
In general, even optimal production schedules tend to be quite degenerate, in the sense that there often exist a large number of different schedules, all of which can achieve a given set of production requirements. However, the potential for heat integration could vary significantly from one such schedule to another. Furthermore, in some industrial sectors (e.g. food, diary, brewing) that employ multipurpose plants, energy costs do form a significant proportion of the total production cost, and thus have to be balanced properly against other costs, such as those of the raw materials and manpower, and the value of the products. On the basis of the above discussion, heat integration must be considered as an integral part of the problem of scheduling the production in a given plant, with the cost of utilities incorporated within the overall economic objective.
In this context, this paper proposes a systematic mathematical framework for the exploitation of heat integration in batch plant operation. The rest of this paper is organized as follow. The next section introduces briefly the *ERTN* formalism and describes the modeling of direct heat integration mode. Then, Section 3 provides a brief review of the proposed formulation. Finally, an example of a heat-integrated process is used to illustrate the approach in section 4.

2. A graphical modelling framework : the *Extended Resource Task Network*

Among the available *CAPE* tools *(Computer Aided Process Engineering)*, process engineers are showing a growing interest in scheduling methods based on *MILP* formulation in order to carry out various performance analyses such as system productivity, time cycle, production costs or energy efficiency of a

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unit. Nevertheless, the implementation and the tuning of a *MILP* model can become rather technical and complex in some cases. To facilitate the modelling phase by non-expert users in optimization, a way is to build mathematical models which are structurally generic and configurable with parameters entered through a well-defined graphical formalism. Provided that the semantic is sufficiently general, it allows the user to describe a problem in an intuitive way while ignoring the mathematical model useful to its resolution. Another advantage of such formalism is the ability to unambiguously model a problem by adding specific construction rules in order to reduces (but it does not avoid) potential modelling mistakes. In this framework, the *Extended Resource Task Network* (*ERTN*) formalism has been developed. Based on the well-known *Resource Task Network* (*RTN*) formalism proposed by (Pantelides, 1994), new semantic elements have been introduced by (Fabre *et al*, 2011) and (Thery *et al*, 2011) in order to handle explicitly cumulative resources (such as utilities for example) and multi-modal resources. *ERTNs* are directed graphs comprising two types of nodes. *State* nodes (denoted by circles) correspond to materials of different types (feeds, intermediate, final products), utilities, waste, device or operator, etc, while *task* nodes (denoted by rectangles) represent physical, chemical or biological transformations of these materials. Different kind of arcs unambiguously represent production procedure (precedence constraints), material and energy flows (ratio of inlet and outlet flows, free flows, mixing and splitting of individual batches, material recycles, shared intermediates) and resource constraints (topology of the unit, capacity of devices, fixed or dependent operating time, shared and multi-modal devices, etc.). Figure 1 summarizes the semantic elements of the *ERTN* formalism.

NOM	SYMBOLE	REPRESENTS
Batch task Node	**T*k* – Operation name** (V_k^{min}, V_k^{max}, pf_k, pv_k, $dd_{r,k}$)	**Discontinuous processing task *k*** the batch size $B_{k,t}$ is such that $V_k^{min} \leq B_{k,t} \leq V_k^{max}$, the processing time is $p_k = pf_k + pv_k B_{k,t}$ and the delivery time of resource r is $dd_{r,k}$ (by default, $dd_{r,k} = p_k$)
Continuous task Node	**T*k* – Operation name** (V_k^{min}, V_k^{max}, pf_k, $dd_{r,k}$)	**Continuous processing task *k*** the flow rate $B_{k,t}$ is such that $V_k^{min} \leq B_{k,t} \leq V_k^{max}$, the processing time is $p_k = pf_k$ and the delivery time of resource r is $dd_{r,k}$ (by default, $dd_{r,k} = 0$)
Cumulative resource Node	**S*r* – Name** ($S0_r$, C_r^{max}) Policy	**Cumulative resource *r*** the amount $S_{r,t}$ of stored resource r is such that $S_{r,t} \leq C_r^{max}$, the initial amount is $S0_r$, the *storage policy* is *UIS* or *NIS* or *FIS* (by default, *FIS*) and the *transfer policy* can be *ZW* (by default, *none*)
Disjuntive resource Node	**Resource Name**	**Disjunctive resource *r*** resource which can be used by only one processing task at a given time
State resource Node	**S*r* - Name** ($S0_r$, C_r^{max}) Policy	**State resource *r*** the amount $S_{r,t}$ is an integer indicating the actual state of the disjunctive resource r. It is such that $S_{r,t} \leq C_r^{max}$, the initial marking is $S0_r$ and the *transfer policy* can be *ZW* (by default, *none*)
Fixed flow Arc	T*k* – Operation name → ($\rho_{k,r}^{prod}$) S*r* – Name ($S0_r$, C_r^{max}) Policy S*r* – Name ($S0_r$, C_r^{max}) Policy → ($\rho_{k,r}^{cons}$) T*k* – Operation name	**Fixed proportion flow of cumulative resource** Cumulative resource flow governed by a conservative mass balance. $\rho_{k,r}^{cons}$ (resp. $\rho_{k,r}^{prod}$) is the fixed proportion of resource r consumed (resp. produced) with respect of $B_{k,t}$ (by default, $\rho_{k,r}^{cons} = 1$ (resp. $\rho_{k,r}^{prod} = 1$))
Free flow Arc	T*k* – Operation name —/→ S*r* – Name ($S0_r$, C_r^{max}) Policy S*r* – Name ($S0_r$, C_r^{max}) Policy —/→ T*k* – Operation name	**Free proportion flow of cumulative resource** Cumulative resource flow governed by a conservative mass balance. The / on arc indicates a free proportion of resource r consumed (resp. produced) with respect of $B_{k,t}$. $\mu_{k,r}^{prod}$ or $\mu_{k,r}^{cons}$ is equal to 1 if a free flow arc exists between cumulative resource r and task k, 0 otherwise.
Production / consumption Arc	S*r* – State ($S0_r$, C_r^{max}) Policy ⇒ ($uf_{k,r}^{cons}$, $uv_{k,r}^{cons}$) T*k* – Operation T*k* – Operation ⇒ ($uf_{k,r}^{prod}$, $uv_{k,r}^{prod}$) S*r* – State ($S0_r$, C_r^{max}) Policy	**Production/consumption flow of cumulative resource** Cumulative resource flow not governed by a conservative mass balance. The produced (resp. consumed) amount of cumulative resource r by task k is $u_{k,r}^{prod} = uf_{k,r}^{prod} + uv_{k,r}^{prod} B_{k,t}$ (resp. $u_{k,r}^{cons} = uf_{k,r}^{cons} + uv_{k,r}^{cons} B_{k,t}$)
Use Arc	Resource Name - - - → T*k* – Operation	**« Use » relationship between a processing task and a disjunctive resource** Indicates that the disjunction resource r has the capability to perform the processing task k.
State transition Arc	T*k* – Operation name -·-→ ($\alpha_{k,r}^{out}$) S*r* - Name ($S0_r$, C_r^{max}) Policy S*r* - Name ($S0_r$, C_r^{max}) Policy -·-→ ($\alpha_{k,r}^{in}$) T*k* – Operation name	**In/out flow of state resource** Indicates an evolution of the actual state (modeled by state resources r) of the disjunctive resource which performes the processing task k. The integer $\alpha_{k,r}^{in} \geq 1$ (resp. $\alpha_{k,r}^{out} \geq 1$) if a transition state arc exists between state resource r and task k, 0 otherwise. By default, $\alpha_{k,r}^{in} = 1$ (resp. $\alpha_{k,r}^{out} = 1$).

Figure 1. Semantic elements of the ERTN graphical formalism

Assuming that the processing equipment available in the plant includes at least one pair of units which are coupled to each other through a heat exchanger, then heat exchange can take place between two processing step that are performed simultaneously in these units. This mode of heat integration is classically denominated by *direct heat integration*. On the basis of the *ERTN* semantic, heat integrated operations are modelled as follow. As we suppose that an heat integrated operation is abble to take place with or without heat integration, each of them are splitted into two tasks *k* and *k'*, one corresponding to the heat-integrated operation and one to the stand-alone operation, as shown in Figure 2. It should be noted that these two tasks involve the same transformation of material, but eventually with different duration and utility consumption. The second issue to be addressed is that of ensuring that a pair of heat-integrated tasks *j* and *k* always start at the same time *t*. For this, a virtual *cumulative resource* node has to be introduced to represent the medium. The *NIS* policy assigned to this state induces that this resource is produced by the task *k* and consumed immediately by the task *j*, thus ensuring the temporal synchronization of the tasks of this couple (see Figure 2). Finally, the ratio *r* of the batch sizes $B_{j,t}$ and $B_{k,t}$ of the heat-integrated tasks *j* and *k* usually has to be fixed in order for their combined operation to be feasible. To ensure this feature, the parameters of the previous production/consumption arcs have to be fixed as shown in Figure 2.

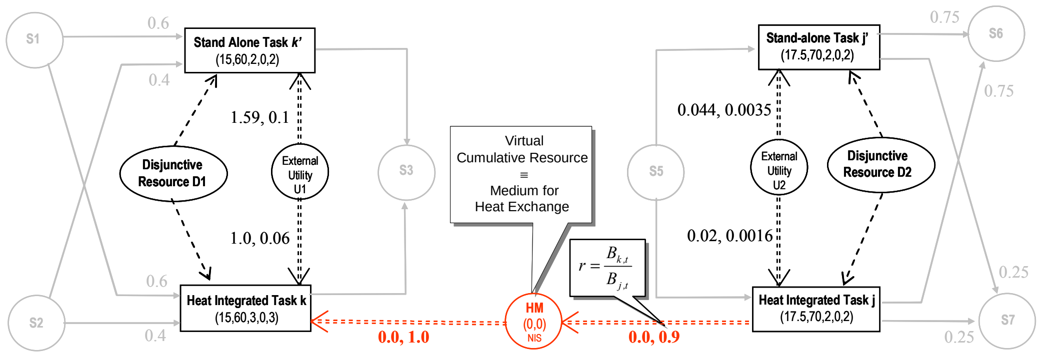

Figure 2. Modeling of Heat Integrated operations

3. Mathematical formulation

Several excellent reviews (Méndez *et al.*,2006), (Floudas & Lin, 2004), (Burkard R.E & Hatzl J., 2005) clearly point out that mixed integer linear programming (*MILP*) has been widely used for solving the batch process scheduling problem. In this framework, various formulations of this problem are proposed in the literature. In this article, a general discrete time *MILP* formulation of the short term scheduling problem under utilities constraints is presented, based on an extension of the *Global time intervals* formulation. In this approach, the time horizon is discretized into a number of intervals of equal duration and system events (task starts and finishes, changes in resource availability, product demands, etc) are allowed to occur only at the boundaries of the time intervals. As stated in section 2, the generic nature of the *ERTN* formalism allows direct correspondence between the semantic structure of the graphical representation and a set of mathematical constraints. The key variables of this formulation are the equipment allocation variables W_{kt} ($W_{k,t} = 1$ if the task *k* is launched at start of period *t* and $W_{k,t} = 0$, otherwise), the batch size variables B_{kt} (defined by the amount or flow rate $I_{r,k,t}$ of resource *r* entering in task *k* and by the amount or flow rate $O_{r,k,t}$ of resource *r* leaving task *k* in period *t*), the amount R_{rt} of cumulative resource *r* stored in period *t*, the production $UO_{r,t}$ or consumption UI_{rt} of cumulative resource *r* in period *t* and finally, the import $In_{r,t}$ and export $Out_{r,t}$ of cumulative resource *r* in period *t*.
The above variables are subject to a number of constraints. Processing equipment allocation constraints (1) express the fact that disjunctive resource *r* ($r \in R^D$) can carry out at most one task *k* ($k \in K_r$) over any given time interval *t*. Constraints (2) define storage capacity of cumulative resource *r* ($r \in R^C$) while processing equipment capacity constraints (3) limits the batch size (resp. flow rate) $B_{k,t}$ that can be undertaken by the batch task $k \in K^B$ (resp. continuous task $k \in K^C$) at time interval *t*. Constraints (4) and (5) are the generalized mass balance applicable for each cumulative resource over time. Note that cumulative resource node can act simultaneously as utility resource and material resource. So, it not only provides the material for a transformation process (acting as material resource through the term $O_{r,k,t}$ and $I_{r,k,t}$) but can also fulfill the utility demands of a processing task (acting as utility resource through the terms $UO_{r,k,t}$ and $UI_{r,k,}$). Moreover, each cumulative resource node can receive resource from external sources (term $In_{r,t}$) and can provide resource to external consumers (term $Out_{r,t}$). Constraints (6) and (7)

fix the minimum and maximum bounds on the imports and exports of cumulative resource r in period t. Orders $D_{r,t}$ of cumulative resource r are taken into account with constraints (8). Constraints (9) and (10) represent the generalized mass balance around the task nodes that transform cumulative resources in known or unknown proportions of batch size (constraints (11) and (12)). Finally, constraints (13) and (14) define production and consumption of cumulative resources).

$$\sum_{k\in K_r}\sum_{\substack{t'=t-p_k+1\\ t>0}}^{t} W_{k,t'} \le 1 \quad \forall r\in R^D, \forall t\in 1,..,T \tag{1}$$

$$0 \le R_{r,t} \le C_r^{max} \quad \forall r\in R^C, \forall t\in 1,..,T \tag{2}$$

$$W_{k,t}V_k^{min} \le B_{k,t} \le W_{k,t}V_k^{max} \quad \forall k\in K, \forall t\in 1,..,T \tag{3}$$

$$R_{r,t} = R_{r,t-1} + \sum_{k\in K^C\cup K^B} O_{r,k,t-dd_{r,k}} - \sum_{k\in K^C\cup K^B} I_{r,k,t} + \sum_{k\in K^C\cup K^B} UO_{r,k,t-dd_{r,k}} - \sum_{k\in K^C\cup K^B} UI_{r,k,t} + In_{r,t} - Out_{r,t} \quad \forall r\in R^C, \forall t\in 1,..,T \tag{4}$$

$$R_{r,0} = R0_r \quad \forall r\in R^C \cup R^S \tag{5}$$

$$Out_{r,t}^{min} \le Out_{r,t} \le Out_{r,t}^{max} \quad \forall r\in R^C \tag{6}$$

$$In_{r,t}^{min} \le In_{r,t} \le In_{r,t}^{max} \quad \forall r\in R^C \tag{7}$$

$$Out_{r,t}^{min} = Out_{r,t}^{max} = D_{r,t} \quad \forall r\in R^C \tag{8}$$

$$B_{k,t} = \sum_{r\in R_k^{cons}} I_{r,k,t} \quad k\in K, \forall t\in 1,..,T \tag{9}$$

$$B_{k,t} = \sum_{r\in R_k^{prod}} O_{r,k,t} \quad k\in K, \forall t\in 1,..,T \tag{10}$$

$$\rho_{k,r}^{prod} B_{k,t} \le O_{r,k,t} \le \left(\rho_{k,r}^{prod} + \mu_{k,r}^{prod}\right) B_{k,t} \quad \forall k\in K, \forall r\in R_k^{prod}, \forall t\in 1,..,T \tag{11}$$

$$\rho_{k,r}^{cons} B_{k,t} \le I_{r,k,t} \le (\rho_{k,r}^{cons} + \mu_{k,r}^{cons}) B_{k,t} \quad \forall k\in K, \forall r\in R_k^{cons}, \forall t\in 1,..,T \tag{12}$$

$$UI_{r,k,t} = \sum_{t'=t-p_k+1}^{t} (uf_{k,r}^{cons} W_{k,t'} + uv_{k,r}^{cons} B_{k,t'}) \quad \forall r\in R^C, \forall k\in K, \forall t\in 1..T \tag{13}$$

$$UO_{r,k,t} = \sum_{t'=t-p_k+1}^{t} (uf_{k,r}^{prod} W_{k,t'} + uv_{k,r}^{prod} B_{k,t'}) \quad \forall r\in R^C, \forall k\in K, \forall t\in 1..T \tag{14}$$

Finally, the objective function takes direct account of the trade-offs between energy savings on one hand, and satisfaction of scheduling constraints (such as timely delivery of orders) on the other. The precise description of these constraints is not important for the purpose of this paper, and the interested reader is referred to the (Agha, 2009) or (Thery *et al*, 2011) paper for more information.

4. Application

In order to demonstre the applicability of the proposed model, we consider a short-term scheduling problem that seeks to determine the optimal utilization of the available plant resources (processing equipment, storage capacity, utilities, etc) over a given time horizon. The multipurpose plant considered is an extension of a classical batch process example used by (Majozi, 2006) or (Chen *et al*, 2008). It consists of a plant manufacturing three products P1, P2 and P3 and production requirements are imposed on them at the end of the horizon. The *generic recipe* includes four operations (*Reaction 1*, *Filtration*, *Distillation* and *Reaction 2*) and the *site recipe* is described by the *ERTN* on Figure 3. Proportions of each material, minimum and maximum batch size, duration of tasks and storage capacity and policy are indicated. Moreover, the processing equipment available in the plant includes two pairs of units which are coupled to each other through a heat exchanger (Reactor 1/Column reboiler and Reactor 1/Reactor 2). Assuming appropriate temperature levels, there is in principle the opportunity of exchanging heat between, on the one hand, the exothermic *Reaction 1* task which requires cooling and the *Distillation* task which requires heating and, on the other hand, the exothermic *Reaction 1* task which requires cooling and the endothermic *Reaction 2* task which requires heating. As mentionned in section 2, these operations have to be splitted in two tasks (SA:*stand-alone* or HI:*heat integrated*). The precise operating mode and heat characteristics of two heat-integrated processing steps taking place in a given pair of equipment items are known. The equipment is also fitted with exchange facilities that allow the use of external utilities (e.g., steam, cooling water) to supplement the heating and cooling loads provided through heat integration. The existence of these additional facilities also makes possible the use of each of the equipment items in a pair for carrying out the corresponding processing step separately, if necessary, i.e. without the need for heat integration. In this context, the processing times of the individual steps when performed separately is different from those for the same steps when heat integration is employed (see Figure 3). In any case, the instantaneous rates of consumption of external utilities over the duration of each step are given on the *ERTN* (see Figure 3).

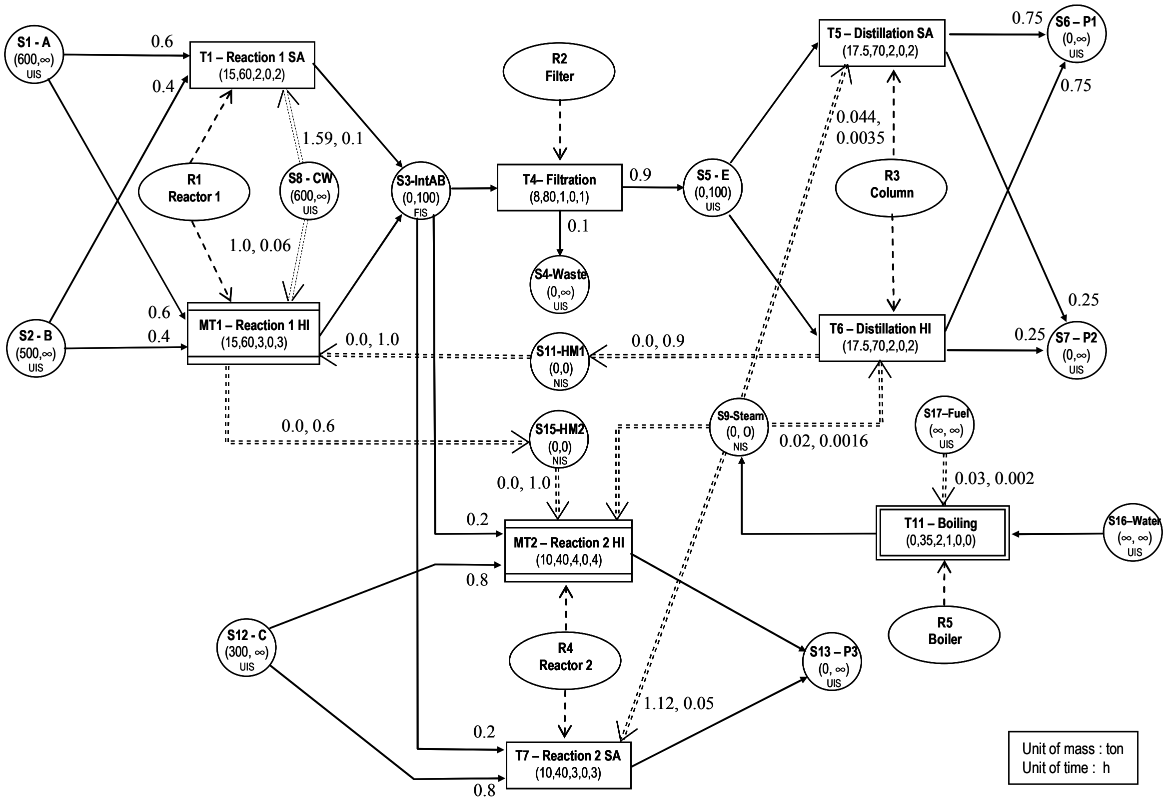

Figure 3. ERTN for example process

Concerning the pair *Reaction 1*/*Distillation,* the heat exchange match would involve task *Reaction 1* being performed in the Reactor 1 and the *Distillation* task in the Column with an offset of 1 h with respect to their starting times. Indeed, such an offset is necessary in order to maximise the potential for heat integration by allowing sufficient time for the *Reaction 1* to reach the operating temperature at which the heat consumed by the *Distillation* is to be generated. Due to the lower temperature differences, the duration of the *Reaction 1* when operated in heat-integrated mode is increased from 2 to 3 hr. As expected, the demands posed by these tasks on external utilities are also modified. So, the macro-task MT1 is decomposed as shown in Figure 4.

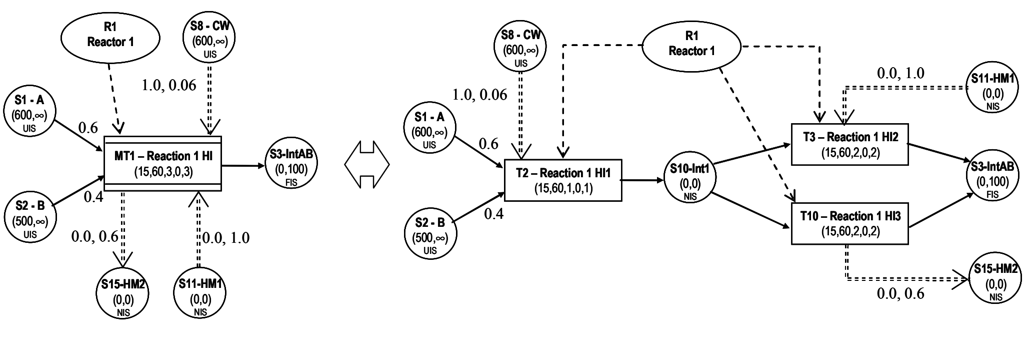

Figure 4. Decomposition of the macro-task MT1

Similar remarks can be made about the pair *Reaction 1*/*Reaction 2.* The heat-integrated *Reaction 1* task always requires a cooling water flow rate of *1.0 + 0.06B t/h* during the first hour of its operation only ;

thereafter all its needs are satisfied through heat exchange with the contents of the Reactor 2. On the other hand, the heat-integrated *Reaction 2* task requires a constant steam flow rate of *0.9+0.031B t/h* during the first two hours (task T8) and a constant steam flow rate of *0.3+0.006B t/h* thereafter (task T9), supplementing the energy received from the heat exchange with the Reactor 1 contents.
Finally, unlimited availability cooling water is assumed. In contrast, steam flow rate is limited and produced by a site utility system (boiling operation T11 that consumes fuel).

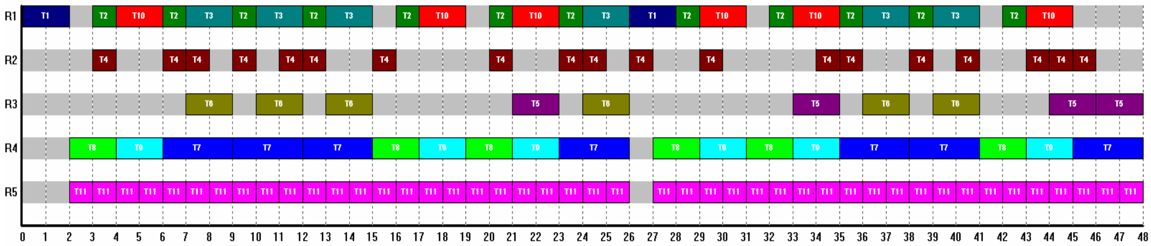

Figure 5. Scheduling corresponding to the manufacturing of 510 t of P1, 170 t of P2 and 300 t of P3

Figure 5 shows the optimal schedule obtained for this problem (solve on a 2.0 GHz Pentium with *XPRESS-MP*) on a time horizon of 48h. The number inside each rectangle in the Gantt chart denotes the task being carried out. It can be seen that this involves both stand-alone operations and integrated ones. Stand-alone tasks are performed sporadically throughout the horizon. This feature of the optimal solution is due to the complex trade-off between increased processing time and reduced utility consumption for the two reaction tasks. Moreover, as expected, heat integrated *Reaction 1* takes place as soon it is possible in order to reduce the consumption of steam of the other integrated operations. Finally, the costs of the utilities consumed are reduced to an even larger extent.

5. Conclusion

This paper has proposed a systematic mathematical framework for the exploitation of heat integration in multipurpose batch plant operation, taking detailed account of its interactions with production scheduling. The *ERTN* formalism has been used to model clearly and unambiguously both the material and utilities flows in the dicontinuous process. Based on this representation, a general scheduling formulation including direct heat integration aspects was examined and an example illustrates the potentiel benefits of this approach. Currently, a *continuous time MILP* formulation and *indirect heat integration* are under consideration.

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